

Localization of Discrete Spectrum of Multiparticle Schrödinger Operators

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An upper bound on the dimension of eigenspaces of multiparticle Schrödinger operators is given. Its relation to upper and lower bounds on the eigenvalues is discussed.

1. Introduction

In the case of one- and two-particle Schrödinger operators H , upper bounds on the multiplicity of eigenvalues have been given in [1–4]. They generalize results of Birman [5], Schwinger [6], and others (for a review see Simon [7]), who gave global bounds on the number of eigenvalues, i.e. bounds on the total number of eigenvalues of H below some $-\kappa^2$, κ positive.

Multiparticle systems admit a wealth of processes, e.g. capture processes, breakup processes, rearrangements and excitations, which cannot occur or occur only rudimentarily in one- and two-particle systems. This dynamical complication is also reflected in the resolvent equation: E.g. the kernel of the homogeneous Lippman-Schwinger equation and the kernel of the Rollnik equation is not compact for particle number N bigger than 2. Therefore a direct transcription to the N particle case is feasible neither for the global bounds [5–7] nor for the local bounds [1–4].

Thus, the results on global bounds on the number of eigenvalues of multiparticle systems appeared relatively late: Yafaev [8] gave bounds on the total number of bound states of some threeparticle systems, whose interaction potentials are short range and negative, using the Faddeev equations. Simon [9] and Klaus and Simon [10] obtained bounds on the total number of eigenvalues for such potentials for the general N -body case, if the essential spectrum of the Schrödinger operator is given by two

cluster breakups. Hill [11–13] has shown, that the H^- -ion has exactly one bound state and that the H^{--} -ion has no bound states at all. The complete absence of bound state for highly negative charged ions in general, i.e. their nonexistence, has been demonstrated by Ruskai [14, 15] and Sigal [16, 17]. In a further step Sigal [16, 18] gave a certain generalization of the Birman-Schwinger principle to the multiparticle case and showed a bound on the number of the eigenvalues of a Schrödinger operator being less than E :

$$\operatorname{tr} |K_1(E)|^2 \cong \dim \{ \varphi \in D(H) \mid \text{ex. } \lambda < E \text{ s. t. } H \varphi = \lambda \varphi \}, \quad (1)$$

where

$$K_1(E) = JK(E)J^{-1}, \quad (J^\delta u)(x) = (1 + |x|^2)^{-\delta/2} u(x)$$

and

$$K(E) = \sum_a J_a R_a(E) W_a. \quad (2)$$

J_a is a Ruelle-Simon partition of unity, R_a is the resolvent of the intercluster Hamiltonian with respect to the cluster decomposition a and

$$W_a = [J_a, -\Delta] + J_a I_a. \quad (3)$$

I_a is the interaction between the clusters of a .

Local bounds on the number of eigenvalues, i.e. bounds on the dimension of $\operatorname{Ker}(H - E)$

$$d(E) = \dim \operatorname{Ker}(H - E), \quad (4)$$

where H is the Schrödinger operator

$$H = \sum_{i=1}^N -\frac{1}{2m_i} \Delta_i + \sum_{\substack{i,j=1 \\ i < j}}^N V_{ij}(x_i - x_j) \quad (5)$$

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reduced on the center of mass system and where E is a negative real number below the bottom of the essential spectrum of H , are unknown. The purpose of the present paper is to give such a bound for a certain class of singular and long-range potentials.

In chapter two we collect some results, which we shall need in the following, and define our notation: The first section of this chapter contains the inequality on the dimension of eigenspaces of operators lying in some trace ideal \mathfrak{T}_{2p} ($p = 1, 2, 3, \dots$); in the second section we give some notations which are useful for describing the breakup of multiparticle systems into clusters, and, furthermore, we show that the trace ideal properties of the symmetrized Weinberg-van Winter kernel depend on the decay properties of the interaction potentials. In chapter three we prove the bound on the dimension of eigenspaces of the Schrödinger operator H using the Weinberg-van Winter equation. In addition we comment on using other integral equations for bound states, e.g. the geometric resolvent equation of Sigal [16, 18]. In chapter four we make explicit the bound of chapter three for the simplest non-trivial system, the helium atom. The concluding chapter five discusses the relation of the bound on the dimension of eigenspaces of H to upper and lower bounds on the eigenvalues of H .

2. Bounds on the Geometric Multiplicity of Eigenvalues and Cluster Decompositions

This chapter collects some results and notations which we shall need in the following:

2.1.: Let \mathfrak{H} be a complex Hilbert space, let H be an element of some trace ideal

$$\mathfrak{T}_{2p} (H \in \mathfrak{T}_{2p} \text{ iff } \operatorname{tr}(|H|^{2p}) < \infty), \quad p = 1, 2, 3, \dots,$$

and z a non zero complex number. Then the following holds:

a) For every $B \in \mathfrak{T}_{2p}$

$$\operatorname{tr}(|[(H-z)B + Hz^{-1}]^p|) \geq \dim \operatorname{Ker}(H-z). \quad (6)$$

b) Set

$$B = \begin{cases} -z^{-1} - ((H-z)|(\operatorname{Ker}(H-z))^\perp)^{-1} \\ -z^{-1} \end{cases} \quad \begin{matrix} \text{on } (H-z)(\mathfrak{H}) \\ \text{on } ((H-z)(\mathfrak{H}))^\perp \end{matrix} \quad (7)$$

Then $B \in \mathfrak{T}_{2p}$ and equality holds in (6).

Proof: See [3].

If one wishes to apply inequality (6) directly by choosing H to be the Schrödinger operator, difficulties arise from the fact that the left hand side does not exist for every trial operator B in \mathfrak{T}_p . In [3] we therefore resorted to an integral equation for the bound states with trace ideal kernel, the Rollnik equation. This is no longer possible for multiparticle systems, since that kernel is no longer compact. There is, however, a substitute for the Rollnik kernel in the case of multiparticle systems which is in some trace ideal \mathfrak{T}_p of finite index p : In the following we shall recapitulate the machinery of the Weinberg-van Winter equation and show trace ideal properties of its kernel.

2.2.: In the following we shall use as far as possible the nomenclature of Simon [19]:

A cluster decomposition D of $\{1, \dots, N\}$ is a family of disjoint subsets of $\{1, \dots, N\}$ whose union is $\{1, \dots, N\}$. The elements of D are called clusters.

Given a cluster decomposition we write iDj , iff i and j are in the same cluster of D , and $\sim iDj$, iff i and j lie in different clusters of D .

$$\text{Let } H = H_0 + \sum_{i < j; i, j=1}^N V_{ij} \text{ be an } N\text{-body Schrö-}$$

dinger operator. Then

$$V_D := \sum_{i, j=1, i < j, iDj}^N V_{ij} \quad (8)$$

is called the cluster potential,

$$H_D := H_0 + V_D \quad (9)$$

the cluster Hamiltonian, and

$$I_D := \sum_{i, j=1, i < j, \sim iDj}^N V_{ij} \quad (10)$$

the intercluster interaction.

Let D_1 and D_2 be two cluster decompositions. D_2 is called a refinement of D_1 , $D_1 \triangleleft D_2$, iff D_2 is obtained from D_1 by further partitioning.

A string S is an ordered family of cluster decompositions $(D_N, D_{N-1}, \dots, D_k)$ with $D_N \triangleright D_{N-1} \triangleleft \dots \triangleright D_k$ such that D_l ($l = k, \dots, N$) contains l elements. We call the string connected, iff $k = 1$. $i(S) := k$ is called the index of the string.

Finally set

$$V_{D_l D_{l-1}} := I_{D_l} - I_{D_{l-1}} = V_{D_{l-1}} - V_{D_l} \quad (11)$$

and

$$R_D := (1 - G_0^{1/2} V_D G_0^{1/2})^{-1}, \quad (12)$$

where $G_0 = (z - H_0)^{-1}$ is the free resolvent. R_D is called the reduced Green's function.

Using these notations, we define the Weinberg-van Winter kernel $I(E)$ to be

$$I(E) = \sum_{S=\{D_N, \dots, D_1\}} (E - H_{D_N})^{-1} V_{D_N D_{N-1}} (E - H_{D_{N-1}})^{-1} \cdot V_{D_{N-1} D_{N-2}} \dots (E - H_{D_2})^{-1} V_{D_2 D_1} \quad (13)$$

(see [19–22]) and the symmetrized Weinberg-van Winter kernel $I_s(E)$ to be

$$I_s(E) = \sum_{S=\{D_N, \dots, D_1\}} (G_0^{1/2} V_{D_N D_{N-1}} G_0^{1/2}) \cdot R_{D_{N-1}} \dots R_{D_2} (G_0^{1/2} V_{D_2 D_1} G_0^{1/2}). \quad (14)$$

In the following for all occurring operators we suppose the center of mass being removed, i.e. we separate out the center of mass motion and choose the configuration space of the N -body system with masses m_1, \dots, m_N to be the hyperplane

$$X = \left\{ x \in \mathbb{R}^{3N} \mid \sum_{i=1}^N m_i x_i = 0 \right\}$$

and define the scalar product in X to be

$$\langle x, y \rangle = 2 \sum_{i=1}^N m_i x_i y_i.$$

In the following we need an integral equation for the bound states whose kernel lies in some trace ideal. Theorem one shows that the symmetrized Weinberg-van Winter kernel yields such an integral equation:

Theorem 1: Let $V_{ij} \in R + L^{2p}(\mathbb{R}^3)$, for some $p = 1, 2, 3, \dots$, and $E < \Sigma$, being the bottom of the essential spectrum of the Schrödinger operator reduced on center of mass coordinates. Then it holds:

- $I_s(E) \in \mathfrak{T}_{2p}(L^2(X))$.
- If H has E as an eigenvalue, then $I_s(E)$ has the eigenvalue one. If ψ is an eigenfunction of H , then

$$(E - H_0)^{1/2} \psi \quad (15)$$

is the corresponding eigenfunction of $I_s(E)$.

Proof: a) The proof is by induction and follows an idea of Hunziker [23] (see also Simon [19], pp. 187). We only have to modify the step from n to $n+1$. We use the notations of Simon [19].

In order to show $I_s(E)$ to be in $\mathfrak{T}_{2p}(L^2(X))$ we consider each individual term of $I_s(E)$ separately, i.e., a general term

$$T = (G_0^{1/2} V_{i_N j_N} G_0^{1/2}) R_{D_{N-1}} (G_0^{1/2} V_{i_{N-1} j_{N-1}} G_0^{1/2}) \dots R_{D_2} (G_0^{1/2} V_{i_2 j_2} G_0^{1/2}), \quad (16)$$

where i_r and j_r are indices in different clusters of D_r but the same cluster of D_{r-1} . Furthermore we introduce the coordinates $x'_k := x_{i_k j_k}$ ($k = 2, \dots, N$), which are a complete independent set of coordinates in X .

We deal with the kernel \mathcal{T} of T in momentum space and prove that

$$\begin{aligned} & \tau(P'_2, \dots, P'_N, \tilde{P}'_2, \dots, \tilde{P}'_N) \\ &= |\mathcal{T}(P'_2, \dots, P'_N, \tilde{P}'_2, \dots, \tilde{P}'_N)| \end{aligned}$$

defines an operator τ such that

$$\tau \in \mathfrak{T}_{2p}(L^2(X)). \quad (17)$$

This implies $T \in \mathfrak{T}_{2p}$.

First we note that

$$T_r = [(G_0^{1/2} V_N G_0^{1/2}) R_{D_{N-1}}] \dots [(G_0^{1/2} V_{r+1} G_0^{1/2}) R_{D_r}], \quad (V_n = V_{i_n j_n}) \quad (18)$$

has no forces between clusters of D_r , so it has a kernel with $\delta(\tilde{P}'_2 - P'_2) \dots \delta(\tilde{P}'_r - P'_r)$, that is

$$\begin{aligned} (T_r f)(P'_2, \dots, P'_N) &= \int d\tilde{P}'_{r+1} \dots \\ &\dots d\tilde{P}'_N \mathcal{T}^{(P'_2, \dots, P'_r)} \cdot (P'_{r+1}, \dots, P'_N, \tilde{P}'_{r+1}, \dots, \tilde{P}'_N) \\ &\quad \cdot f(P'_2, \dots, P'_r, \tilde{P}'_{r+1}, \dots, \tilde{P}'_N). \end{aligned} \quad (19)$$

Let $t_r^{(P'_2, \dots, P'_r)}$ be the operator which has the absolute value of $\mathcal{T}^{(P'_2, \dots, P'_r)}$ as kernel. We shall show inductively that the $\mathfrak{T}_{2p}(L^2(P'_{r+1}, \dots, P'_N))$ -norm is uniformly bounded in P'_2, \dots, P'_r ; i.e. there exists a d_r such that for all P'_2, \dots, P'_r

$$\|t_r^{(P'_2, \dots, P'_r)}\|_{\mathfrak{T}_{2p}(L^2(P'_{r+1}, \dots, P'_N))} < d_r < \infty. \quad (20)$$

Start the induction with $r = N$ so $\mathcal{T}_N^{(P'_2, \dots, P'_N)} = 1$. Clearly $t_N^{(P'_2, \dots, P'_N)}$ fulfills (20).

Now, suppose we know $t_r^{(P'_2, \dots, P'_r)}$ obeys the claim. Let $S_r^{(P'_2, \dots, P'_{r-1})}$ be the operator which has the

absolute value of the kernel of $T_r(G_0^{1/2} V_r G_0^{1/2})$ as kernel:

$$\begin{aligned} & \mathcal{A}_r^{(P'_2, \dots, P'_{r-1})} (P'_r, \dots, P'_N, \tilde{P}'_r, \dots, \tilde{P}'_N) \\ &= |\mathcal{T}_r^{(P'_2, \dots, P'_r)} (P'_{r+1}, \dots, P'_N, \tilde{P}'_{r+1}, \dots, \tilde{P}'_N) \\ & \cdot G_0^{1/2} (P'_2, \dots, P'_r, \tilde{P}'_{r+1}, \dots, \tilde{P}'_N) \hat{V}_r (P'_r - \tilde{P}'_r) \\ & \cdot G_0^{1/2} (P'_2, \dots, P'_{r-1}, \tilde{P}'_r, \dots, \tilde{P}'_N)|, \end{aligned} \quad (21)$$

where \hat{V}_r is the suitably normalized Fourier transform of V_r and

$$G_0^{1/2} (P'_2, \dots, P'_N) = -i (\Sigma a_{ij} P'_i P'_j - E)^{-1/2}, \quad (22)$$

where a_{ij} is a positive definite matrix. Since a'_{ij} is positive definite we can find $C > 0$ such that

$$\Sigma a_{ij} P'_i P'_j \geq C \Sigma P_i'^2. \quad (23)$$

Thus

$$|G_0^{1/2} (P'_2, \dots, P'_N)| \leq |C P_r'^2 - E|^{-1/2}. \quad (24)$$

As a result,

$$\begin{aligned} & \mathcal{A}_r^{(P'_2, \dots, P'_{r-1})} (P'_r, \dots, P'_N, \tilde{P}'_r, \dots, \tilde{P}'_N) \\ & \leq |\mathcal{T}_r^{(P'_2, \dots, P'_r)} (P'_{r+1}, \dots, P'_N, \tilde{P}'_{r+1}, \dots, \tilde{P}'_N)| \\ & |C P_r'^2 - E|^{-1/2} |\hat{V}_r (P'_r - \tilde{P}'_r)| |C \tilde{P}_r'^2 - E|^{-1/2}. \end{aligned} \quad (25)$$

We now decompose the potential $V_r = V'_r + V''_r$ in a part $V'_r \in R$ and a part $V''_r \in L^{2p}(\mathbb{R}^3)$. Let

$$\begin{aligned} W_f(P'_r, \tilde{P}'_r) &= |C P_r'^2 - E|^{-1/2} \\ & \cdot \hat{f}(P'_r - \tilde{P}'_r) |C \tilde{P}_r'^2 - E|^{-1/2}. \end{aligned}$$

$W_{V'_r}$ is Hilbert-Schmidt (Simon [19], p. 22). Using Russo's inequality (Simon [24], p. 57)

$$\|K\|_q \leq (\|K\|_{q', q} \|K^*\|_{q', q})^{1/2}, \quad (26)$$

where K is an integral operator with kernel $K(x, y)$ and $\|K\|_{r, s} = (\int (\int |K(x, y)|^r dx)^{s/r} dy)^{1/s}$ and $K^*(x, y) = \overline{K(y, x)}$, we get

$$\begin{aligned} \|W_{V''_r}\|_{2p} & \leq \{[\int dy |Cy^2 - E|^{-p} (\int dx |\hat{V}''_r|^{(2p)'}) \\ & \cdot (y-x) |Cx^2 - E|^{-(2p)'/2} 2p/(2p)']^{1/(2p)} \\ & \cdot [\int dx |Cx^2 - E|^{-p} (\int dy |\hat{V}''_r|^{(2p)'}) \\ & \cdot (x-y) |Cy^2 - E|^{-(2p)'/2} 2p/(2p)']^{1/(2p)}\}^{1/2} \\ & \leq |E|^{-p} \|V''_r\|_{(2p)'} * |c x^2 - E|^{-(2p)'/2} \| \cdot \|_{2p/(2p)'}^{1/(2p)'} \\ & \leq |E|^{-p} \| \hat{V}''_r \|_{(2p)'} \|c x^2 - E\|^{-1/2} \| \cdot \|_{2p}^{1/2p} < \infty \end{aligned} \quad (27)$$

(c some positive constant), where we used Young's inequality to estimate the norm of the convolution. Combining the trace ideal properties of $W_{V'_r}$ and $W_{V''_r}$ yields $W_{V_r} \in \mathfrak{T}_{2p}$. Thus

$$\begin{aligned} & \|S_r^{(P'_2, \dots, P'_{r-1})}\|_{\mathfrak{T}_{2p}(L^2(P'_r, \dots, P'_N))} \\ & \leq \int d^3(N-r+1) P^{(1)} \dots d^3(N-r+1) P^{(2p)} \\ & \cdot | [W_{V_r}(P_r^{(2)} - P_r^{(1)}) | \mathcal{T}^{(P'_2, \dots, P'_{r-1}, P_r^{(2)})} (P'_{r+1}, \dots, P'_N, \\ & \quad P_r^{(1)}, \dots, P_r^{(1)}) | \\ & \quad | \mathcal{T}^{(P'_2, \dots, P'_{r-1}, P_r^{(2)})} (P'_{r+1}, \dots, P'_N, P_{r+1}^{(3)}, \dots, P_N^{(3)}) | \\ & \quad \cdot W_{V_r}(P_r^{(2)} - P_r^{(3)})] \\ & \quad : \\ & \cdot [W_{V_r}(P_r^{(2p)} - P_r^{(2p-1)}) \\ & \quad | \mathcal{T}^{(P'_2, \dots, P'_{r-1}, P_r^{(2p-1)})} (P'_{r+1}, \dots, P_N^{(2p)}, \\ & \quad P_{r+1}^{(2p-1)}, \dots, P_N^{(2p-1)}) | \\ & \quad \mathcal{T}^{(P'_2, \dots, P'_{r-1}, P_r^{(2p)})} (P'_{r+1}, \dots, P_N^{(2p)}, P_{r+1}^{(1)}, P_N^{(1)}) | \\ & \quad \cdot W_{V_r}(P_r^{(2p)} - P_r^{(1)})] \} \\ & \leq \| [(t_r^{(P'_2, \dots, P'_{r-1}, P_r^{(1)})}) * t_r^{(P'_2, \dots, P'_{r-1}, P_r^{(2)})}] \\ & \quad \cdot [(t_r^{(P'_2, \dots, P'_{r-1}, P_r^{(2p-1)})}) * \\ & \quad \cdot t_r^{(P'_2, \dots, P'_{r-1}, P_r^{(2p)})}] \|_{\mathfrak{T}_1(L^2(P'_{r+1}, \dots, P'_N))} \\ & \quad \cdot \|W_{V_r}\|_{\mathfrak{T}_1(L^2(P'_r))}^{2p} \\ & \leq \prod_{i=1}^{2p} \|t_r^{(P'_2, \dots, P'_{r-1}, P_r^{(i)})}\|_{\mathfrak{T}_{2p}(L^2(P'_{r+1}, \dots, P'_N))} \\ & \quad \cdot \|W_{V_r}\|_{\mathfrak{T}_1(L^2(P'_r))}^{2p} \leq d_r^{2p} \|W_{V_r}\|_{\mathfrak{T}_{2p}(L^2(P'_r))}. \end{aligned} \quad (28)$$

Thus, the existence and uniform boundedness in P'_2, \dots, P'_{r-1} of the \mathfrak{T}_{2p} -norms of $S_r^{(P'_2, \dots, P'_{r-1})}$ -follows. Now $t_r^{(P'_2, \dots, P'_{r-1})} = S_r^{(P'_2, \dots, P'_{r-1})} R_{D_{r-1}}$ and $R_{D_{r-1}}$ has $\delta(\tilde{P}'_2 - P'_2) \dots \delta(\tilde{P}'_{r-1} - P'_{r-1})$ in its kernel, since x'_2, \dots, x'_{r-1} are intercluster coordinates. R_{D_r} considered as a family of operators on $L^2(P'_r, \dots, P'_N)$ has a uniformly bounded operator norm (uniform in P'_2, \dots, P'_{r-1}). Thus $t_r^{(P'_2, \dots, P'_{r-1})}$ has uniformly bounded \mathfrak{T}_{2p} -norms. This completes the induction.

b) See Reed and Simon [25], p. 344.

We remark that the theorem has an obvious transcription to the unsymmetrized Weinberg-van Winter kernel. We have to require the potentials V_{ij} to be in $L^2(\mathbb{R}^3) + L^{2p}(\mathbb{R}^3)$ ($p = 1, 2, \dots$) in this case.

3. Upper Bound on the Dimension of Eigenspaces of Schrödinger Operators

Using the Weinberg-van Winter equation, its trace ideal properties and its relation to the bound states, we get the following result:

Theorem 2: Let $E < \Sigma$ and $V_{ij} \in R + L^{2p}(\mathbb{R}^3)$. Then

$$\begin{aligned} g(E) &= \text{tr} |(I_s(E) - 1) B + I_s(E) \mathcal{P}|^2 \\ &\geq \dim \text{Ker}(H - E). \end{aligned} \quad (30)$$

Furthermore for

$$B = \begin{cases} -1 - ((I_s(E) - 1) \| (\text{Ker}(I_s(E) - 1))^\perp)^{-1} \\ -1 \end{cases} \quad \text{on} \quad \begin{matrix} (I_s(E) - 1)(L^2(X)) \\ ((I_s(E) - 1)(L^2(X)))^\perp \end{matrix} \quad (31)$$

the left hand side of (30) is minimal.

Proof: Follows from (6) and (7) and the trace ideal properties of the symmetrized Weinberg-van

Winter equation and its relation to the bound states of H .

Remarks:

a) It is not necessary that the operator B as defined in (31) yields equality in (30); but choosing this B , the left hand side of (30) can only be greater than the right hand side for a particular E , if $I_s(E)\psi = \psi$ has a “spurious” solution, i.e. $I_s(E)$ has the eigenvalue one, but H reduced on the center of mass frame does not have E as an eigenvalue. This situation can actually occur (see Federbush [26]). One could circumvent this difficulty by using instead of the symmetrized Weinberg-van Winter kernel some other kernel, e.g. the Faddeev-Yakubovskii kernel [27, 28], which does not have spurious solutions. Given some trace class properties of the Faddeev-Yakubovskii kernel it is easy to transcribe theorem two to this case. Nevertheless we do not follow this way because of notational economy. (The Faddeev-Yakubovskii kernel is a matrix-integral kernel.) An other possibility would be to use the operator K_1 of Sigal (equation one) instead of the Weinberg-van Winter kernel.

b) Our bound has an obvious transcription to the case where one uses the unsymmetrized Weinberg-van Winter kernel instead of the symmetrized one. In this case one has to require $V_{ij} \in L^2(\mathbb{R}^3) + L^{2p}(\mathbb{R}^3)$.

c) We can also handle systems with external forces as long as the corresponding potentials V_i are in $R + L^{2p}(\mathbb{R}^3)$ (or $L^2(\mathbb{R}^3) + L^{2p}(\mathbb{R}^3)$). The Hamiltonian of such an N -particle system has the same form as an $N + 1$ -particle Hamiltonian reduced on the center of mass frame except that the matrix a_{ij} (see (21)) is not diagonal in the latter case, which is unessential.

d) It is also possible to handle restrictions due to permutational symmetries of the systems. One can e.g. use the modification of the Weinberg-van Winter kernel by Balslev [29] instead of $I(E)$ or $I_s(E)$.

4. Explicit Bounds for Coulomb Systems

The bounds of chapter three contain the reduced resolvents R_D . In order to make them explicit we have to have some knowledge about the kernel of reduced resolvents. We shall give explicit expressions for these kernels in the case of the simplest multiparticle Coulomb system, the helium atom in Born-Oppenheimer approximation. The corresponding Schrödinger operator is

$$H(x) = -\Delta_1 - \Delta_2 - r_1^{-1} - r_2^{-1} + \alpha r_{12}^{-1}, \quad (32)$$

where $\alpha = 1/Z$ with Z the charge of the nucleus (Thirring [30], p. 191). We can use the unsymmetrized form of the Weinberg-van Winter kernel because the singular part of the Coulomb potential is square integrable. It reads (Thirring [30], p. 220)

$$\begin{aligned} I(E) = & (E - H_0)^{-1} r_1^{-1} (E - H_0 + r_1^{-1})^{-1} \\ & \cdot (-r_2^{-1} + \alpha r_{12}^{-1}) \\ & + (E - H_0)^{-1} r_2^{-1} (E - H_0 + r_2^{-1})^{-1} \\ & \cdot (-r_1^{-1} + \alpha r_{12}^{-1}) \\ & + (E - H_0)^{-1} \alpha r_{12}^{-1} (E - H_0 - \alpha r_{12}^{-1})^{-1} \\ & \cdot (r_1^{-1} + r_2^{-1}). \end{aligned} \quad (33)$$

Because of the Born-Oppenheimer approximation H_0 is just the six dimensional Laplacian. Thus

$$(E - H_0)^{-1}(p, p') = \delta(p - p') (E - p^2)^{-1}. \quad (34)$$

The potentials occurring in (33) are explicitly known. The only operators whose integral kernels are not at hand, are the reduced resolvents in (33). In order to give an explicit kernel for these terms we first note that $(E - H_0 - \alpha/r_1)^{-1}$ is the only occurring type of reduced resolvent. The two other terms, especially $(E - H_0 + \alpha/r_{12})^{-1}$, can be brought into this form by change of variables.

In momentum space the operator $E - H_0 - a/r_1$ becomes

$$(E - p^2) \delta(p - p') - \left(\frac{a}{r_1} \right) (p_1 - p'_1) \delta(p_2 - p'_2). \quad (35)$$

Thus

$$(E - H_0 - a/r_1)^{-1} (p_1, p_2, p'_1, p'_2) = \delta(p_2 - p'_2) \cdot (Z + A - a/r_1)^{-1} (p_1, p'_1) |_{Z=E-p_2^2}. \quad (36)$$

Now, using the integral representation for the one-particle Coulomb Green's function (Schwinger [31]), we get

$$(E - H_0 - a/r_1)^{-1} (p, p') = \delta(p_2 - p'_2)$$

$$\cdot \left\{ \frac{\delta(p_1 - p'_1)}{E - p^2} + \frac{a}{8\pi^2(E - p_2^2)} \int_0^1 d\varrho \, \varrho^{ia/(4\sqrt{E - p_2^2})} \cdot \frac{1 - \varrho^2}{[(p_1 - p'_1)^2 \varrho - (1 - \varrho)^2 (E - p^2) (E - p'^2)/(4(E - p_2^2))]^2} \right\} \quad (37)$$

which is the last step in making the Weinberg-van Winter kernel explicit in the case of the helium atom.

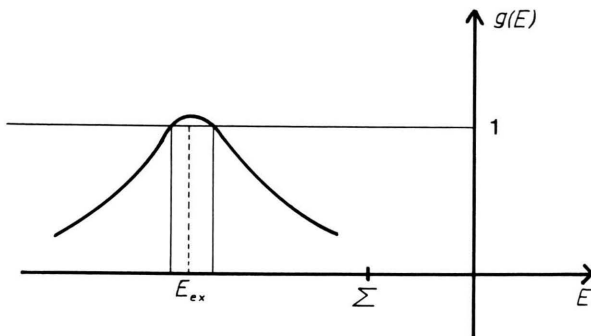


Fig. 1. Construction of upper and lower bounds to an eigenvalue E_{ex} of multiplicity one below the bottom of the essential spectrum Σ .

5. Upper and Lower Bounds on the Eigenvalues

As in the oneparticle case, the bound on the dimension of eigenspaces can be used to localize the eigenvalues of the Schrödinger operator below the bottom of the essential spectrum (see [3, 32]): Eigenvalues can only occur where the bound is bigger or equal to one, i.e. the eigenvalues are necessarily in between the points where $g(E)$ drops below one. In order to get a localization of the eigenvalues it is necessary to choose the trial operator B sufficiently near to the minimal operator

(31). In principle this could be done by using a Fredholm series for B . But due to high dimension of the configuration space it is more convenient to choose

$$B = \sum_{n,m=1}^M \alpha_{n,m} |e_n\rangle \langle e_m|, \quad (38)$$

where e_n are suitably chosen orthonormal functions and where the coefficients $\alpha_{n,m}$ are chosen such that $g(E)$ becomes minimal. The functions e_n and the coefficients $\alpha_{n,m}$ may depend on the parameter E .

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